Temperature Dependence of Hall Response in Doped Antiferromagnets

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Using finite-temperature Lanczos method the frequency-dependent Hall response is calculated numerically for the t-J model on the square lattice and on ladders. At low doping, both the high-frequency $R_{\rm H}^*$ and the d.c. Hall coefficient $R_{\rm H}^0$ follow qualitatively similar behavior at higher temperatures: being hole-like for $T > T_s$!$\approx$!$1.5J$ and weakly electron-like for $T < T_s$. Consistent with experiments on cuprates, $R_{\rm H}$ changes, in contrast to $R_{\rm H}^*$, again to the hole-like sign below the pseudogap temperature T^*, revealing a strong temperature variation for $T \to 0$.

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The anomalous behavior of the Hall constant $R_{\rm H}$ in the normal state of cuprates [1] remains the challenge for theoreticians for over a decade. Two aspects, possibly interrelated, are evident and should be understood: a) the d.c. $R_{\rm H}^0$ at low temperatures $T \to 0$ is clearly doping dependent. In the prototype material $\mathrm{La}_{2-x}\mathrm{Sr}_x\mathrm{CuO}_4$ (LSCO) it changes from positive $R_{\rm H}^0 \propto 1/x$ at low doping $x < x^* \approx 0.3$, consistent with the picture of hole-doped (Mott-Hubbard) insulator, to the electron-like $R_{\rm H}^0 < 0$ at $x > x^*$ in agreement with the usual band picture. b) $R_{\rm H}^0$ is also strongly temperature dependent, both at low doping and optimum doping. At optimum doping, the attention has been devoted to the anomalous variation of the Hall angle $\theta_{\rm H} \propto T^2$ in $\mathrm{YBa_2Cu_3O_7}$ [2]. On the other hand, at low hole concentration $c_h < 0.15$, $R_{\rm H}(T)$ in LSCO has been shown to follow an universally behaved [3] decrease with T in which $R_{\rm H}^0(T\to 0)$ and the characteristic temperature T^* of vanishing $R_{\rm H}^(T^*) \sim 0$ both scale with c_h. In underdoped cuprates, the same $T^*(c_h)$ has been in fact associated with the (large) pseudogap crossover scale in uniform susceptibility $\chi_0(T)$, in-plane resistivity $\rho(T)$, specific heat $c_v(T)$, and some other quantities [4].

A number of theoretical investigations have addressed the first question, i.e. the doping dependence of $R_{\rm H}$ in models of strongly correlated electrons, in particular within the t-J model and the Hubbard model on a planar lattice. The advantage is that one can study the dynamical Hall response and the d.c. Hall constant as a ground state ($T = 0$) property, in particular in systems with finite transverse dimension [5, 6] and in the ladder geometry [7, 8]. It has been also shown that within the t-J model the change from a hole-like to an electron-like Hall response can be qualitatively reproduced by studying the high-frequency $R_{\rm H}^* = R_{\rm H}(\omega\to\infty)$ [11], analytically tractable at $T \to \infty$. Recently, a connection of the reactive $R_{\rm H}^0(T{=}0)$ to the charge stiffness has also been found [9].

The anomalous temperature dependence of $R_{\rm H}(T)$, being the main subject of this work, has been much less clarified in the literature, The Hall mobility $\mu_{\rm H}(T)$ of a single charge carrier in the Mott-Hubbard insulator has been first evaluated within the generalized retraceable path approximation [10]. The high-frequency $R_{\rm H}^*(T)$ has been calculated using the high-T expansion [11]. At low doping, $c_h < 0.15$, it has been observed that on decreasing temperature $R_{\rm H}^*$ is also decreasing instead of approaching presumed (larger) semiclassical and experimentally observed d.c. result $R_{\rm H}^c = 1/c_h e_0 \approx 4R_{\rm H}^*(T=\infty)$. Related are the conclusions of the quantum Monte-Carlo study of the planar Hubbard model [12], where close to the half-filling electron-like $R_{\rm H}^* < 0$ has been found at low T. The same has been claimed generally for $R_{\rm H}(\omega)$ even for low ω [12]. Quite controversial are also results for $R_{\rm H}^0(T)$ on ladders [7]. In regard to that, we should also mention the questionable relation of the off-diagonal σ_{xy} to the orbital susceptibility χ_d [6, 13], potentially useful as an alternative route to the understanding of $R_{\rm H}^0(T)$ [14].

In the following we present numerical results for the dynamical $R_{\rm H}(\omega)$, as obtained within the low doping regime of the t-J model using the finite-temperature Lanczos method (FTLM) [15, 16]. The aim of this letter is to approach the low-ω and low-T limit as much as possible and to investigate the relation between $R_{\rm H}^*(T)$ and $R_{\rm H}^0(T)$. We find these two quantities essentially different for $T < T^*$, establishing the pseudogap scale $T^* < J$ both in the ladder and planar systems.

We study the t-J model in an external homogeneous magnetic field $\mathbf{B} = \mathrm{curl}\,\mathbf{A}$,

$$H(\mathbf{A}) = -\,t \sum_{\langle ij\rangle s} (\mathrm{e}^{\mathrm{i}\theta_{ij}} \tilde{c}_{is}^\dagger \tilde{c}_{js} + \mathrm{H.c.}) + \\ + J \sum_{\langle ij\rangle} (\mathbf{S}_i\cdot\mathbf{S}_j - \tfrac{1}{4} n_i n_j), \qquad (1)$$

where the (inhomogeneous) vector potential enters the phases $\theta_{ij} = e\mathbf{A}(\mathbf{r}_i)\cdot\mathbf{r}_{ij}$. The hopping is only between the nearest neighbors $\langle ij\rangle$. Projected fermionic operators $\tilde{c}_{is}$, $\tilde{c}_{is}^\dagger$ do not allow for the double occupancy of sites.

In order to calculate the dynamical Hall coefficient

$$R_{\rm H}(\omega) = \frac{\partial \rho_{xy}(\omega)}{\partial B}\Big|_{B\to 0} = \frac{\sigma_{xy}(\omega)}{B\sigma_{xx}(\omega)\sigma_{yy}(\omega)}\Big|_{B\to 0}, \qquad (2)$$

the conductivity tensor is evaluated within the linear response

theory,

$$\sigma_{\alpha\beta}(\omega) = \frac{\mathrm{i}e^2}{N\omega^+}\left[\langle\tau_{\alpha\beta}\rangle - \mathrm{i}\int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\langle[j_\alpha(t), j_\beta]\rangle\right], \quad (3)$$

where in the presence of $B \neq 0$ the particle current $\mathbf{j}$ and the stress tensor $\underline{\tau}$ operators are given by

$$\mathbf{j} = t\sum_{\langle ij\rangle s}\mathbf{r}_{ij}(\mathrm{i}\mathrm{e}^{\mathrm{i}\theta_{ij}}\tilde{c}^\dagger_{is}\tilde{c}_{js} + \mathrm{H.c.}),$$
$$\underline{\tau} = t\sum_{\langle ij\rangle s}\mathbf{r}_{ij}\otimes\mathbf{r}_{ij}(\mathrm{e}^{\mathrm{i}\theta_{ij}}\tilde{c}^\dagger_{is}\tilde{c}_{js} + \mathrm{H.c.}). \quad (4)$$

On a square lattice with N sites and periodic boundary conditions (b.c.) one cannot apply arbitrary magnetic field B since only quantized $B = B_m = m\Phi_0 a^2/N$ can be made compatible with the periodic b.c. [12]. Therefore the smallest but finite $B = B_1$ is used in calculations. The square lattices used are in general Euclidean (tilted) $N = l^2 + n^2$, in particular we investigate systems $N = 10$, 16, 18. On the other hand, the ladder geometry of $N = L \times M$ sites with the periodic b.c. in the L direction and open b.c. in the perpendicular M direction allows for any finite $B \neq 0$, the fact already used in several $T = 0$ calculations [5, 6, 8]. The advantage of ladder systems is also the existence of the reference ground-state results $R^0_{\mathrm{H}}(T{=}0)$ which seem to be better understood [8, 9]. Furthermore, at low doping they reproduce the simple semiclassical behavior $R^0_{\mathrm{H}}(T{=}0) \sim R^{\mathrm{c}}_{\mathrm{H}} = 1/c_h e_0$.

Dynamical components $\sigma_{\alpha\beta}(\omega)$ are evaluated using the FTLM [15], employed so far for various dynamic and static quantities within the t-J model [16], among them also the $B = 0$ optical conductivity $\sigma(\omega) = \sigma_{\alpha\alpha}(\omega)$ on a square lattice. Comparing to the diagonal $\sigma_{\alpha\alpha}$, the evaluation of the off-diagonal $\sigma_{xy}(\omega)$ is more demanding for several reasons: a) the introduction of $B > 0$ in the model (1) breaks the translational invariance and prevents the reduction of the basis states in the Lanczos procedure, hence available finite-size systems are somewhat smaller, b) we expect $\sigma_{xy}(\omega) \propto B$ while $\sigma_{xy}(B{=}0, \omega)$ does not vanish identically within the FTLM; consequently larger sampling over initial wavefunctions [15, 16] are needed to reduce the statistical error, c) on a finite square lattice the reference result $R^0_{\mathrm{H}}(T{=}0)$ is not meaningful for $B_m > 0$, while in ladder systems it is quite sensitive to the introduction of an additional flux [8]. Nevertheless, in general, restrictions for the validity of the FTLM results are similar to other quantities. Through the thermodynamic partition function $Z(T_{\mathrm{fs}}) = Z^*$, we can define the marginal finite-size T_{fs} below which too few levels contribute to the average and results loose the thermodynamic validity [16]. In the following, we analyze results for $J = 0.4t$ at low hole doping $c_h = N_h/N$ ($N_h = 1$, 2). In this regime we can estimate $T_{\mathrm{fs}}/t \sim 0.15 - 0.2 \lesssim 0.5J/t$.

Let us first present results for the dynamical $R_{\mathrm{H}}(\omega)$. In Fig. 1 we show the normalized real part $r_{\mathrm{H}} = e_0 c_h \,\mathrm{Re}\, R_{\mathrm{H}}$ for systems with a single hole $N_h = 1$. In the evaluation of $R_{\mathrm{H}}(\omega)$ from Eq. (2) we insert complex $\sigma_{\alpha\alpha}$ at $B = 0$ and

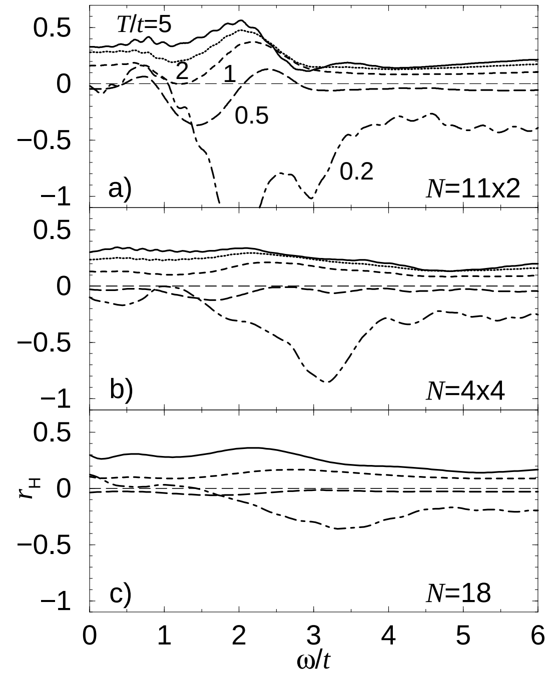

Figure 1: Dynamical Hall response $r_{\mathrm{H}}(\omega) = e_0 c_h \,\mathrm{Re}\, R_{\mathrm{H}}(\omega)$ for different temperatures T/t and various systems with a single hole $N_h = 1$: a) 2-leg ladder with $L = 11$, b) 4-leg ladder with $L = 4$, and c) square lattice with $N = 18$ sites.

the most sensitive quantity remains $\sigma_{xy}(\omega)$ calculated at $B = B_1$ on a square lattice and $B \sim 0.3B_1$ on ladders. In the presentation of results an additional frequency smoothening $\delta = 0.2t$ is used. The normalization of R_{H} is chosen such that at low doping $r_{\mathrm{H}} = 1$ would show up in the case of the semiclassical result.

In Fig. 1 several common features of R_{H} in the ladder geometry and in the 2D systems are recognized:
a) $r_{\mathrm{H}}(\omega)$ is quite smoothly varying function of ω, at least in contrast to strongly ω-dependent $\mathrm{Re}\,\sigma(\omega)$ on a 2D system, which is found [16] to decay with an anomalous relaxation rate $1/\tau(\omega) \propto \omega + \xi T$.
b) At high temperatures $T > t$ we get a hole-like $r_{\mathrm{H}} > 0$ for all systems. In this regime $r_{\mathrm{H}}(\omega)$ is very smooth, in particular for the $M = 4$ ladder and the 2D lattice.
c) For low temperatures $T < t$, $r_{\mathrm{H}}(\omega)$ is less smooth and the dependence is more pronounced for the 2-leg ladder. On the other hand, $M = 4$ ladder clearly approaches the behavior of the 2D system, whereby both of the latter show quite a modest variation of $r_{\mathrm{H}}(\omega)$. In all systems the resonances (and the variation) visible in $r_{\mathrm{H}}(\omega)$ at high $\omega > t$ reflect the predominantly local physics of the hole motion and are thus not related to a current relaxation rate deduced from $\sigma(\omega)$.

Results for $r_{\mathrm{H}}(\omega)$ are the basis for the calculation of high-frequency $r^*_{\mathrm{H}} = r_{\mathrm{H}}(\omega{=}\infty)$ as well as the d.c. limit $r^0_{\mathrm{H}} = r_{\mathrm{H}}(\omega{\to}0)$. The latter is more sensitive since in a finite system (even at $T > 0$) $\sigma_{\alpha\beta}(\omega{\to}0)$ can be singular due to the coherent charge transport in a system with periodic b.c.. The coherent transport shows up in a finite (but small) charge stiffness [16],

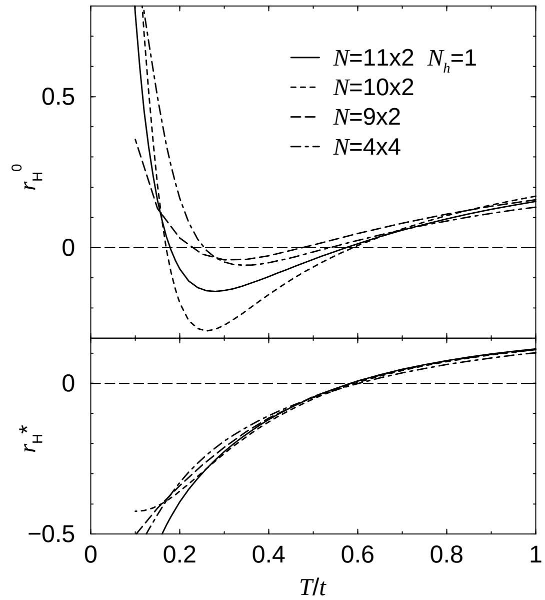

Figure 2: D.c. Hall constant r_{H}^0 and the infinite-frequency r_{H}^* vs. T/t for various ladders $L \times M$ with a single hole $N_h = 1$.

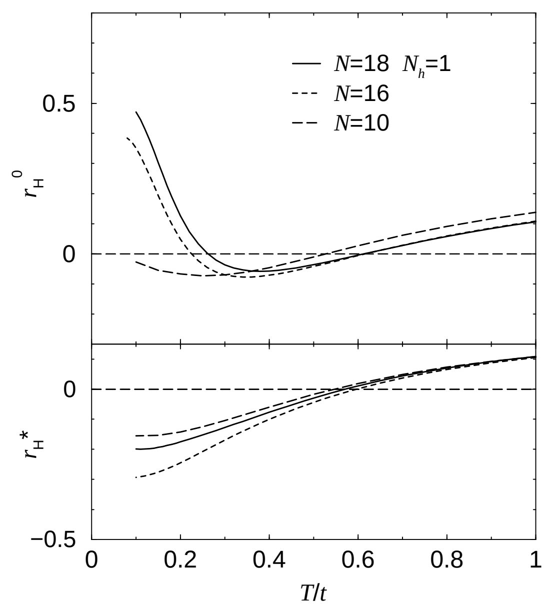

Figure 3: r_{H}^0 and r_{H}^* vs. T/t for different square lattices with N sites and a single hole $N_h = 1$.

which should be omitted in the evaluation of Eq. (2). In any case, one should take into account proper $\omega \to 0$ behavior of dissipative systems at $T > 0$ which is different in ladders and in 2D lattices, respectively: a) On a ladder we get in the leading order of $\omega \to 0$ a normal conductance along the x-direction, i.e. $\sigma_{xx}(\omega \to 0) \sim \sigma_0$, but a finite polarizability along the y-direction, $\sigma_{yy}(\omega{\to}0) \propto \omega\chi_{yy}^0$. Hence, we expect $\sigma_{xy} \propto \omega$ and finite r_{H}^0. b) For a macroscopic isotropic 2D system we get $\sigma_{\alpha\alpha}(\omega{\to}0) \to \sigma_0$ and we expect as well $\sigma_{xy} \to \sigma_{xy}^0$, leading to finite r_{H}^0.

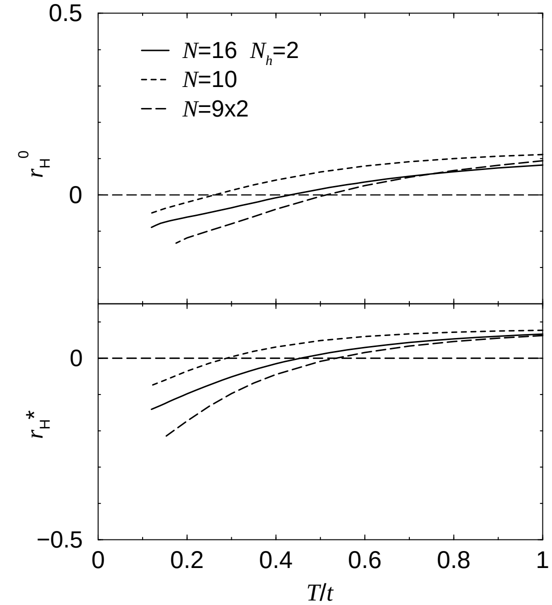

Figure 4: r_{H}^0 and r_{H}^* vs. T/t for different square and ladder lattices with N sites and $N_h = 2$.

In Fig. 2 we present results for $r_{\mathrm{H}}^*(T)$ and $r_{\mathrm{H}}^0(T)$ for the ladder systems with $N_h = 1$. Results are shown for 2-leg ladders with various lengths $L = 9$, 10, 11 and for $M = 4$ ladder with $L = 4$. Since r_{H}^0 and r_{H}^* are properly scaled, for given M curves are expected to approach a well defined macroscopic limit at $L \to \infty$. In fact, r_{H}^* are nearly independent of L (as well as of M) down to $T \sim T_{\mathrm{fs}}$. A crossover at $T_s \sim 0.6t$ from a hole-like $r_{\mathrm{H}}^* > 0$ into a electron-like $r_{\mathrm{H}}^* < 0$ can be explicitly observed. r_{H}^0 results are more size (L) dependent, nevertheless they reveal a crossover nearly at the same $T \sim T_s$. In contrast to r_{H}^* which remains negative for the whole regime $T < T_s$, r_{H}^0 changes sign again at $T{=}T^* \sim 0.2t$. Although our data for T^* are more scattered the crossover into the hole-like $r_{\mathrm{H}}^0(T{<}T^*) > 0$ is expected. Namely, from the ground state calculations in same systems [8] we know that $r_{\mathrm{H}}^0(T{=}0) \sim 1.5$ and $r_{\mathrm{H}}^0(T{=}0) \sim 1.2$ for $M = 2$ and $M = 4$ ladders, respectively. Therefore, it is not surprising that the observed dependence $r_{\mathrm{H}}^0(T{<}T^*)$ is very steep.

Corresponding results for the planar lattice in Fig. 3 are both qualitatively and quantitatively similar. Note, that at low doping the limiting value $r_{\mathrm{H}}^*(T{\to}\infty) = 1/4$ agrees with the analytical result [11], while obtained $r_{\mathrm{H}}^0(T{\to}\infty) \sim 0.3$ is also quite close. Again, the crossover into an electron-like regime appears at $T_s \sim 0.6t$. For larger sizes $N \geq 16$ the lower crossover $T^* \sim 0.2t$ is visible as well. In finite 2D systems a reference numerical result at $T = 0$ does not exist, however, the analytical theory [17] indicates that in a macroscopic limit with a single hole ($N_h = 1$) in an ordered antiferromagnet one should get $r_{\mathrm{H}}^0 = 1$.

In numerically available systems, $N_h = 2$ represents already a substantial doping. Therefore, results for r_{H}^0 and r_{H}^*

shown in Fig. 3 should be interpreted in relation with the corresponding finite doping c_h. Main message of Fig. 3 is that upper crossover T_s, still nearly the same in both $r^0_{\rm H}(T)$ and $r^*_{\rm H}(T)$, shifts down quite systematically with increasing c_h, i.e. with decreasing size N at given N_h. At least in ladder systems at $c_h < 0.3$, we still find $r^0_{\rm H}(T=0) > 0$ in the ground state [8], therefore also the lower crossover $T^* < T_s$ is expected. However, we cannot detect such a crossover in $r^0_{\rm H}(T)$ down to $T_{\rm fs} \sim 0.15t$, not surprisingly since also the experimental value, e.g. in LSCO at $c_h > 0.1$, is $T^* < 600\,{\rm K} \sim 0.15t$ (assuming $t \sim 0.4\,e{\rm V}$).

Let us finally comment on the relation of the d.c. σ^0_{xy} to the orbital susceptibility χ_d in a macroscopic 2D system. Namely, $\tilde{\sigma}^0_{xy} = eB\partial\chi_d/\partial\mu = eB(\partial\chi_d/\partial c_h)(\partial c_h/\partial\mu)$, (where μ denotes chemical potential) was derived using seemingly quite general thermodynamic relations [6, 13], but at the same time put under question [6]. Since the d.c. $\sigma^0_{\alpha\alpha}(T) > 0$ is quite a smooth function the above relation seems to yield also a qualitative connection between $\chi_d(T)$ and $R^0_{\rm H}(T)$. The situation should be particularly simple at low doping (but not too low T), where $\partial c_h/\partial\mu \sim c_h/T$ and $\chi_d \propto c_h$ is expected, and consequently $\tilde{\sigma}_{xy} \propto -B\chi_d/T$. Indeed, results for $N_h = 1$ indicate [14] that both crossovers T_s and T^* appear also as a change of sign in $\chi_d(T)$ nearly at the same values. Here, the intermediate regime $T^* < T < T_s$ corresponds to an anomalous paramagnetic response $\chi_d > 0$. On the other hand, it is quite evident from our results that the relation is not valid at high $T \gg t$. Namely, in this regime $\sigma^0_{\alpha\alpha} \propto 1/T$ and $\sigma^0_{xy} \propto B/T^2$ [10] is obtained, leading to $R^0_{\rm H}(T\to\infty) \sim$ const. On the other hand, from the high-T expansion $\chi_d \propto 1/T^3$ is acquired [14], so that the assumed relation would demand $\tilde{\sigma}^0_{xy} \propto B/T^4$, in conflict with previous $\sigma^0_{xy} \propto B/T^2$.

In conclusion, we have presented results for both dynamical and d.c. Hall constant within the t-J model on ladders and on square lattices. The main novel point is the observation of two crossover temperatures T_s and T^* which are at low doping generally present in all systems. Both $R^*_{\rm H}$ and $R^0_{\rm H}$ are positive at $T > T_s$ and change sign at T_s. While $R^*_{\rm H}(T<T_s)$ stays negative, $R^0_{\rm H}$ reveals a sign change into a hole-like behavior at $T=T^* < T_s$ as well as steep variation of $R^0_{\rm H}(T<T^*)$. This reconciles some seemingly controversial theoretical results [11, 12]. Our results are in agreement with high-T expansion results for $R^*_{\rm H}(T)$ which at low c_h also show decreasing positive values with decreasing T. Quantum Monte Carlo results within the Hubbard model for $R_{\rm H}({\rm i}\omega)$ correspond effectively to high (imaginary) frequencies and low T, and being negative they are in agreement with our findings for $R^*_{\rm H}$.

How should we understand the above numerical results? At high $T \gg t$ and low doping $c_h \ll 1$, $R^*_{\rm H}$ as well as $R^0_{\rm H}$ are governed by a loop motion (that is where the dependence on $B \neq 0$ comes from) of a hole within a single plaquette [10, 11]. One expects $R^*_{\rm H} > 0$, but $r^*_{\rm H} = 1/4$ is a non-universal value which e.g. depends on the lattice coordination [11]. The electron-like $r^*_{\rm H}(T=0) < 0$ represents an instantaneous Hall response within the ground state near half filling is harder to explain, but is clearly the signature of strong correlations. On the other hand at low T, $R^0_{\rm H}$ tests the (low energy) quasiparticle properties. Evidently, at low doping and $T < T^*$ at least a single hole in an antiferromagnetic spin background behaves as a well defined hole-like quasiparticle leading to $r^0_{\rm H}(T\to 0) \sim 1$ both in 2D [17] and in ladders [8]. Our results for vanishing $R^0_{\rm H}(T^*) \sim 0$ indicate that the quasiparticle character is essentially lost at quite low $T \sim T^* < J$, with the pseudogap scale $T^*(c_h)$ decreasing with doping. Such phenomenon is possibly consistent with the scenario of electrons being effectively composite particles (spinons and holons) in strongly correlated systems [2, 19], at least at $T > T^*(c_h)$, whereby $T^*(c_h)$ vanishes at optimum doping.

Finally, let us note that our results for $R^0_{\rm H}$ are in several aspects consistent with experiments on cuprates, and with LSCO in particular. At low doping $c_h < 0.1$ we find $T^* \sim J/2$, close to the observed $T^* \sim 800\,{\rm K}$. At the same time, we find a very steep dependence in $R^0_{\rm H}(T<T^*)$. With increasing c_h, $T^*(c_h)$ seems to have desired decreasing tendency, although to establish this beyond a reasonable doubt more work is needed.

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